

Simultaneous optimization of mechanical properties of steel by maximizing exponential desirability functions

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Summary. A modelling approach to optimize a multiresponse system is presented. The approach aims to identify the setting of the input variables to maximize the degree of overall satisfaction with respect to all the responses. An exponential desirability functional form is suggested to simplify the desirability function assessment process. The approach proposed does not require any assumptions regarding the form or degree of the estimated response models and is robust to the potential dependences between response variables. It also takes into consideration the difference in the predictive ability as well as relative priority among the response variables. Properties of the approach are revealed via two real examples — one classical example taken from the literature and another that the authors have encountered in the steel industry.

Keywords: Desirability function; Fuzzy logic; Multiresponse system; Simultaneous optimization

1. Introduction

Response surface methodology (RSM) consists of a group of techniques used in the empirical study of the relationship between the response and a number of input variables. Consequently, the experimenter attempts to find the optimal setting for the input variables that maximizes (or minimizes) the response. A second-order polynomial model, along with least squares fitting, is widely used to study such an empirical relationship. For detailed information on the various techniques used in RSM, see Box and Draper (1987) and Khuri and Cornell (1996). Most of the work in RSM has been focused on the case where there is only one response of interest. A common problem in product or process design, however, is the selection of optimal parameter levels, which involve the simultaneous consideration of multiple-response variables, called a multiresponse problem.

Multiresponse problems are quite prevalent across various application areas. One typical example that the authors have encountered in the steel industry is as follows. The mechanical properties of hot rolled steel strips are determined by the composition of the steel and processing parameters. The purpose of the study was to determine the effects of steel composition as well as rolling and cooling conditions — the percentage of carbon x_1 , the percentage of

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manganese x_2 , the percentage of silicon x_3 , the thickness of the strips or plates x_4 , the milling temperature x_5 and the coiling temperature x_6 — on the mechanical properties of the JS-SS400-type steel. The mechanical properties were measured by three different responses — the tensile strength y_1 , the yield strength y_2 and the elongation y_3 . The tensile strength is a nominal-the-best (NTB) type of response, whereas the yield strength and elongation are larger-the-better (LTB) types of response.

Various attempts have been made to model such relationships since the 1950s (Kwon and Baik, 1989). The assessed relationships are used in adjusting the composition of the steel and the electrical and mechanical settings for hot rolling and subsequent cooling conditions to obtain the desired property balancing. However, it is not easy to optimize the balance between the mechanical properties. The problem arises because the three responses (especially y_1 and y_3) tend to increase or decrease together, but y_1 is an NTB-type and y_2 and y_3 are LTB-type responses. Moreover, the responses cannot be directly compared because y_3 is measured in a different unit (in per cent) from y_1 or y_2 (in kilograms per millimetre squared). Most of the past attempts have considered only one property (i.e. the tensile strength) in making such adjustments. This was mainly due to the lack of a systematic way of simultaneously considering all the responses, even though the overall quality is defined by the balance between all three properties. With customers' expectations of better quality and market competitiveness, the company realizes that the ability to improve their steel quality by better balancing the responses is crucial for their survival. This example presents a typical situation in many industrial problems involving improvements in the process.

A brief review of previous developments in multiresponse optimization is given in Section 2. The framework of the modelling approach proposed is introduced in Section 3. In Section 4, the classical example from Khuri and Conlon (1981) is used to compare our approach with the generalized distance approach. Section 5 discusses the assessment of the exponential desirability function, a major component of the modelling approach proposed, and its sensitivity analysis. The problem from the steel industry introduced above will be discussed in detail in Section 6. A modified modelling approach to accommodate the difference in the predictive ability among responses is presented in Section 7. Finally, conclusions are made in Section 8. The data that are analysed in this paper can be obtained from

<http://www.blackwellpublishers.co.uk/rss/>

2. Literature review

The multiresponse problem consists of roughly three stages: data collection (the design of experiments), model building and optimization. We shall focus on the optimization issue in this work, assuming that the data have been collected and suitable models have been fitted. One popular approach to simultaneously optimizing (strictly speaking, compromising) multi-responses has been the use of a dimensionality reduction strategy. This method converts a multiresponse problem into a problem with a single aggregate measure and solves it as a single objective optimization problem. The single aggregate measure has often been defined as a desirability function (Harrington, 1965; Derringer and Suich, 1980) or an estimated distance from the ideal design point (Khuri and Conlon, 1981). In this paper, we propose an alternative formulation to such approaches based on maximizing exponential desirability functions.

Suppose that there are r responses $\mathbf{y} = (y_1, y_2, \dots, y_r)$ which are determined by a set of input variables $\mathbf{x} = (x_1, x_2, \dots, x_p)$. A general multiresponse problem can be defined as

$$y_j = f_j(x_1, x_2, \dots, x_p) + \epsilon_j, \quad j = 1, 2, \dots, r,$$

where f_j denotes the response function between the j th response and the input variables and ϵ_j is a random error. The exact form of f_j is usually unknown, but it can be estimated over a limited experimental region by using model building techniques such as regression.

One simple and intuitive approach to a multiresponse problem is to superimpose the response contour plots and to determine an 'optimal' solution by a visual inspection (Lind *et al.*, 1960). The usefulness of such a method is severely limited by the number of input variables and/or responses. The next two subsections briefly review the two most prominent methods in this field, namely the desirability function approach and the generalized distance approach.

2.1. Desirability function approach

The desirability function approach transforms an estimated response (e.g. the j th estimated response \hat{y}_j) to a scale-free value d_j , called desirability. It is a value between 0 and 1, and increases as the desirability of the corresponding response increases. The overall desirability D , another value between 0 and 1, is defined by combining the d_j using a geometric mean (Harrington, 1965):

$$D = (d_1 d_2 \dots d_r)^{1/r}. \quad (1)$$

Then the objective is to find the input variable setting \mathbf{x}^* which maximizes the value of D .

Derringer and Suich (1980) extended Harrington's approach by suggesting a more systematic transformation scheme from \hat{y}_j to d_j . Later, Derringer (1994) suggested a new form of D using a weighted geometric mean:

$$D = (d_1^{w_1} d_2^{w_2} \dots d_r^{w_r})^{1/\sum w_j}, \quad (2)$$

where the w_j are relative weights among the r responses, $j = 1, 2, \dots, r$. If all the w_j are set to 1, equation (2) reduces to equation (1). The value of D does not allow a clear interpretation, except the principle that a higher value of D is preferred. As an example, if the overall desirability D at \mathbf{x}_1 , $D(\mathbf{x}_1)$, is higher than $D(\mathbf{x}_2)$, then \mathbf{x}_1 is considered a better design point than \mathbf{x}_2 , but it is generally impossible to assign a physical meaning to the desirability values $D(\mathbf{x}_1)$ and $D(\mathbf{x}_2)$ as well as the difference $D(\mathbf{x}_1) - D(\mathbf{x}_2)$.

2.2. Generalized distance approach

Khuri and Conlon (1981) proposed an algorithm for the optimization of a multiresponse system based on the generalized distance concept. They first obtained individual optima of the estimated responses over the experimental region and then found the compromised optimum by minimizing the distance function by measuring the deviation from the ideal optimum. They proposed several distance measures ρ including

$$\rho\{\hat{\mathbf{y}}(\mathbf{x}), \phi\} = \{(\hat{\mathbf{y}}(\mathbf{x}) - \phi)' \hat{\Sigma}^{-1}(\hat{\mathbf{y}}(\mathbf{x}) - \phi)/\mathbf{z}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}(\mathbf{x})\}^{1/2}, \quad (3)$$

where $\phi = (\phi_1, \phi_2, \dots, \phi_r)'$ is the ideal optimum, $\hat{\Sigma}$ is the estimator of the common variance-covariance matrix of the random errors ($\epsilon_1, \epsilon_2, \dots, \epsilon_r$), \mathbf{X} is the design matrix and $\mathbf{z}(\mathbf{x})$ is a column vector of the input variables of the given model. Their work also takes into consideration the variation caused by the randomness of ϕ by minimizing an upper bound on the distance within the confidence region of ϕ . A similar idea was also

given by Church (1978) who used the Euclidean distance between $\hat{y}(\mathbf{x})$ and ϕ instead of equation (3).

This method is statistically sound in that the proposed distance measure considers the deviation from the ideal point and accounts for the variances and correlations of the responses. However, it makes rather rigid assumptions (e.g. all response functions depend on the same set of input variables and are of the same form—second-order polynomials) which would restrict its applicability in a general situation. For example, including the extra explanatory variables with zero coefficients may cause problems in routine optimization procedures, such as creating a zero denominator. Furthermore, this approach does not consider the difference in the predictive ability (or goodness of fit) of the estimated response models. When such a difference is not negligible, the results from this approach can be misleading (as will be discussed in Section 7).

3. Optimization scheme proposed

We propose an alternative formulation to the conventional desirability function approach for the multiresponse problem based on maximizing desirability functions. As in the conventional desirability function approach, it is assumed that the degree of satisfaction of the experimenter (or decision maker (DM)) with respect to the j th response variable is maximized when $\hat{y}_j(\mathbf{x})$ equals its target value T_j and decreases as $\hat{y}_j(\mathbf{x})$ moves away from T_j . If y_j^{\min} and y_j^{\max} respectively represent the lower and upper bounds of aspirations, the DM does not accept a solution \mathbf{x} for which $\hat{y}_j(\mathbf{x}) \leq y_j^{\min}$ nor for which $\hat{y}_j(\mathbf{x}) \geq y_j^{\max}$. Thus the degree of satisfaction with respect to the response can be modelled by a function which decreases monotonically from 1 at $\hat{y}_j(\mathbf{x}) = T_j$ to 0 at $\hat{y}_j(\mathbf{x}) \leq y_j^{\min}$ or $\hat{y}_j(\mathbf{x}) \geq y_j^{\max}$.

3.1. Desirability function of a response

For a simple illustration, it is assumed that the degree of satisfaction changes linearly as a function of $\hat{y}_j(\mathbf{x}) - T_j$ for the time being. The desirability function value of a response, denoted $d_j\{\hat{y}_j(\mathbf{x})\}$ ($j = 1, 2, \dots, r$), can then be expressed as in Fig. 1(a):

$$d_j\{\hat{y}_j(\mathbf{x})\} = \begin{cases} 0, & \text{if } \hat{y}_j(\mathbf{x}) \leq y_j^{\min} \text{ or } \hat{y}_j(\mathbf{x}) \geq y_j^{\max}, \\ 1 - \frac{T_j - \hat{y}_j(\mathbf{x})}{T_j - y_j^{\min}}, & \text{if } y_j^{\min} < \hat{y}_j(\mathbf{x}) \leq T_j, \\ 1 - \frac{\hat{y}_j(\mathbf{x}) - T_j}{y_j^{\max} - T_j}, & \text{if } T_j \leq \hat{y}_j(\mathbf{x}) < y_j^{\max}. \end{cases} \quad (4)$$

This procedure can be easily modified for the smaller-the-better (STB) or LTB type of situation. Setting $y_j^{\min} = T_j = 0$ (assuming that $\hat{y}_j(\mathbf{x})$ is non-negative) represents the STB case, whereas setting $y_j^{\max} = T_j$ at a sufficiently large value represents the LTB-type situation. (See Fig. 1(b) for the desirability function of an STB-type response.) A non-linear-shaped desirability function can also be employed. (See Fig. 1(c).) The determination of a desirability function shape will be further discussed in Section 5.

3.2. Determination of bounds

As discussed above, the bounds on a response (y_j^{\min} and y_j^{\max}) should be specified to define the desirability function. The bounds may be determined on the basis of the specification limits of the product or process, regulations or standards of the organization or the DM's subjective

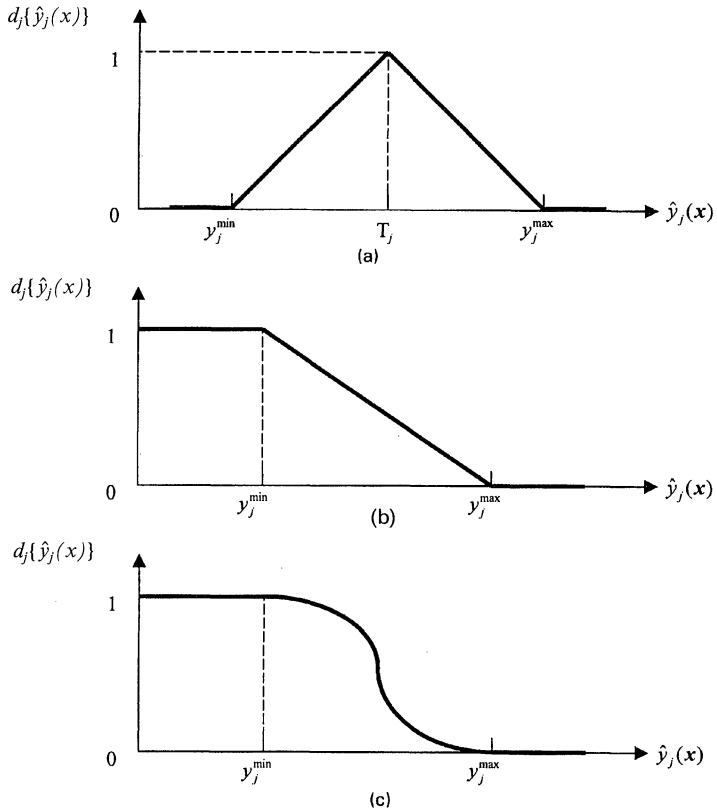


Fig. 1. Desirability functions of $\hat{y}_j(x)$: (a) NTB type and linear case; (b) STB type and linear case; (c) STB type and non-linear case

judgments. If it is desirable to determine the bounds on the basis of the physical range of the response and if the response surface has been ‘reasonably fully explored’, they can be set at the extreme values of the individual estimated response:

$$y_j^{\min} = \min_{x \in \Omega} \{\hat{y}_j(\mathbf{x})\}, \tag{5}$$

$$y_j^{\max} = \max_{x \in \Omega} \{\hat{y}_j(\mathbf{x})\}. \tag{6}$$

The bounds determined by equations (5) and (6) represent the minimum and maximum possible values of the estimated response within the experimental region Ω .

3.3. Formulation

A multiresponse problem requires an overall optimization, i.e. simultaneous satisfaction with respect to all the response variables. If a ‘minimum’ operator is employed for aggregating the responses, a multiresponse optimization problem can be stated as

$$\text{maximize } \lambda \tag{7}$$

subject to

$$d_j\{\hat{y}_j(\mathbf{x})\} \geq \lambda, \quad j = 1, 2, \dots, r, \quad (8)$$

$$\mathbf{x} \in \Omega. \quad (9)$$

This formulation aims to identify \mathbf{x}^* which maximizes the minimum degree of satisfaction (λ) with respect to all the responses within the experimental region, i.e.

$$\underset{\mathbf{x} \in \Omega}{\text{maximize}} (\min [d_1\{\hat{y}_1(\mathbf{x})\}, d_2\{\hat{y}_2(\mathbf{x})\}, \dots, d_r\{\hat{y}_r(\mathbf{x})\}]).$$

Additional constraints may be added to this formulation as appropriate. The formulation can be extended to cope with the situation where two or more of the responses were alternatives rather than all being essential. This could be done by employing a ‘maximum’ operator (i.e. by taking the maximum of their degrees of satisfaction).

3.4. Discussion

The optimization scheme proposed above has several methodological advantages over the existing methods. First, the proposed ‘maximin’ approach is robust to the potential dependences between responses. Such dependence is very difficult to detect or model in reality. Dependence can appear in various forms, whereas a pairwise linear relationship is probably the only case that can possibly be detected. When the assumption of independence is violated, both the conventional desirability function approach (using the average or weighted average to aggregate the individual desirability values) and the generalized distance approach can be very misleading, as noted by Khuri and Conlon (1981). The procedure proposed, however, focuses on the response which has the lowest degree of satisfaction, and thus the inequalities in expression (8) corresponding to other responses are essentially redundant constraints from the optimization viewpoint. It is well known in the optimization literature that redundant constraints do not play any role in determining the optimal solution (Murty, 1976). Therefore, the existence of dependence between responses does not affect the procedure proposed.

Secondly, the approach proposed achieves a better balance between all the responses compared with the existing methods. Optimizing a single aggregate measure— D (given in equation (1) or (2)) in the conventional desirability function approach or ρ (given in equation (3)) in the generalized distance approach—does not explicitly consider the balance between the multiple conflicting responses and thus may result in a setting \mathbf{x} at which the outcome on some of the responses is not acceptable. The approach proposed first specifies practically allowable ranges on each of the responses and then maximizes the overall satisfaction level within the ranges in such a way that the contribution of each response is properly reflected in the optimization. (This point will be demonstrated through an example in Section 4.)

Thirdly, the objective function value λ allows a good physical interpretation. The λ -value denotes the overall degree of satisfaction ($0 \leq \lambda \leq 1$) based on the specified ranges of all the responses. It can be used as a basis for a meaningful comparison between different design points. A design point \mathbf{x}_1 is preferred to another design point \mathbf{x}_2 if $\lambda(\mathbf{x}_1) > \lambda(\mathbf{x}_2)$. Moreover, $\lambda(\mathbf{x}_1) - \lambda(\mathbf{x}_2)$ represents how much \mathbf{x}_1 is preferred to \mathbf{x}_2 in terms of the overall degree of satisfaction, which was not possible with the aggregated desirability value D of the conventional desirability function approach. Finally, the approach proposed can be easily understood and implemented by those with little mathematical or statistical knowledge, possibly with the aid of a software system.

It should also be noted that the proposed maximin approach has possible disadvantages as well. In particular, the approach proposed only considers the response with the lowest degree

of satisfaction, and thus the degrees of satisfaction associated with all other responses are, in effect, ignored. This may lead to an unreasonable decision in some cases. As an extreme example, the approach would prefer an operating set-up with $(d_1, d_2, d_3, d_4) = (0.5, 0.5, 0.5, 0.5)$ to that with $(d_1, d_2, d_3, d_4) = (0.99, 0.99, 0.99, 0.49)$. It is thus recommended to perform several approaches for the final decision, unless the DM surely understands that this scenario is invalid. Furthermore, the dependences between responses can be viewed as a source of extra information. The fact that the approach is insensitive to dependences means that it does not utilize such information in the data.

It is worth noting that the approach proposed can also be viewed as a fuzzy logic approach. Specifically, the approach adopts two concepts which also exist in fuzzy logic: the desirability function (as a special case of the membership function) and the fuzzy 'and' operator. Conceptually, a desirability function can be considered a special case of a membership function in fuzzy set theory in the sense that the desirability value of an estimated response is in essence the grade of membership to a fuzzy set representing the 'ideal' response (Chameau and Santamarina, 1987). The proposed maximin approach is equivalent to using the logical and operator in fuzzy logic, denoting the intersection of the corresponding membership functions. This optimization scheme has been proven to be useful, in the fuzzy logic literature, to compromise multiple conflicting objectives (Bellman and Zadeh, 1970; Zimmermann, 1987). For a discussion on the use of fuzzy methods in statistical problems, see Laviolette *et al.* (1995). In the remainder of this paper, we shall focus on the generalized distance approach as a reference method against which our proposed approach is compared.

4. Example 1: texture characteristic study

The classical example from Khuri and Conlon (1981) is employed to illustrate the approach proposed and to compare it with the generalized distance approach. The purpose of the experiment was to determine the effects of cysteine (x_1) and calcium chloride (x_2) on the texture characteristics of a dialysed whey protein concentrates gel system. The texture characteristics were measured by hardness y_1 , cohesiveness y_2 , springiness y_3 and 'compressible water' y_4 , all of which were LTB-type responses. The experimental region was a circle of radius $\sqrt{2}$ centred at the origin. The experiment was conducted in a central composite design with five centre points. A second-order model was fitted to each of the four responses (see Table 2 on page 368 of Khuri and Conlon (1981)). For a fair comparison with Khuri and Conlon's (1981) results, the full second-order model is used, although some items are clearly insignificant. The minimum and maximum values y_j^{\min} and y_j^{\max} of each individual fitted response were obtained, as discussed in equations (5) and (6): $(y_j^{\min}, y_j^{\max}) = (0.37, 2.68), (0.30, 0.69), (1.10, 1.90), (0.23, 0.71)$ for $j = 1, 2, 3, 4$ respectively. These values were used as the bounds on each response. The target value T_j is set equal to y_j^{\max} ($j = 1, 2, 3, 4$) because all the responses are to be maximized.

The desirability function of each response, $d_j\{\hat{y}_j(\mathbf{x})\}$, is defined as in equations (4). A linear desirability function is employed for simplicity. (The issues associated with the shape of the desirability function will be discussed further in Section 5.) The results of the approach proposed are summarized and compared with those of Khuri and Conlon (1981) (referred to as the KC approach) in Table 1.

The KC and the proposed approaches yield different optimal settings, $\mathbf{x}^* = (x_1, x_2) = (-0.46, -1.38)$ compared with $(0.35, -1.37)$, and consequently different ρ^* and λ^* . As expected, \mathbf{x}^* from the KC approach has a better (smaller) ρ^* , whereas \mathbf{x}^* from the approach proposed has a better (higher) λ^* . In the KC approach, $\hat{y}_1(\mathbf{x}^*)$, $\hat{y}_2(\mathbf{x}^*)$ and $\hat{y}_3(\mathbf{x}^*)$ are not too different from their corresponding individual maxima, as manifested by the relatively high

Table 1. Comparison of results: KC approach *versus* the approach proposed

Parameter	Results for the KC approach	Results for the approach proposed
Optimal setting \mathbf{x}^*	(-0.46, -1.38)†	(0.35, -1.37)
Predicted response value $\hat{y}_j(\mathbf{x}^*)$	(2.47, 0.54, 1.83, 0.31)	(1.68, 0.55, 1.62, 0.50)
Desirability function value $d_j\{\hat{y}_j(\mathbf{x}^*)\}$	(0.92, 0.62, 0.90, 0.16)	(0.57, 0.65, 0.65, 0.57)
Distance measure $\rho^*\dagger$	14.69	21.42
Overall degree of satisfaction $\lambda^*\ddagger$	0.16	0.57

†Obtained by using the distance measure defined by equation (3) (which corresponds to equation (4.4) in Khuri and Conlon (1981), page 366).

‡ $\lambda^* = \min_j\{d_j\{\hat{y}_j(\mathbf{x}^*)\}\}$.

$d_j\{\hat{y}_j(\mathbf{x}^*)\}$ values (0.92, 0.62 and 0.90, for $j = 1, 2, 3$ respectively). However, y_4 has been sacrificed; $\hat{y}_4(\mathbf{x}^*)$ is only 0.31 with $d_4\{\hat{y}_4(\mathbf{x}^*)\}$ being 0.16, which essentially defines the overall degree of satisfaction. The desirability values from the approach proposed show that, compared with the KC approach, a significantly *better* balance between the responses is attained with the overall degree of satisfaction of 0.57. Of course, as previously mentioned, the meaning of ‘better’ depends on the detailed nature of the problem.

The KC approach assumes that all responses have the same functional form (a second-order polynomial, in particular). This is not required in the approach proposed. If the best subset model (rather than the full second-order model) were used for each response, the optimal setting would be $\mathbf{x}^* = (0.31, -1.38)$ with $\hat{y}(\mathbf{x}^*) = (1.77, 0.56, 1.64, 0.47)$ and $\lambda^* = 0.55$. Non-linear fittings, if so desired, can easily be incorporated in our procedure. A formal comparison with the KC approach will be presented in Section 7 (Table 3).

5. Desirability function assessment

The approach proposed requires that the desirability function of each response be specified. A linear desirability function (e.g. those in Figs 1(a) and 1(b)) is defined by fixing the lower and upper levels of acceptability (and a target value in the NTB case). It can serve as an approximation to the exact form of the desirability functions when the system is insensitive to the shape of the desirability function. See, for example, Inglis *et al.* (1997) for a case in biology, where the output from the fuzzy model using linear functions differed little from that obtained by using normal distribution functions.

When a non-linear desirability function is desired, the process of selecting an admissible functional form is difficult and time consuming. However, it can be simplified by employing a general functional form which can generate a rich variety of shapes by adjusting its parameters. In view of this, we suggest the use of an exponential function of the form

$$d(z) = \begin{cases} \frac{\exp(t) - \exp(t|z|)}{\exp(t) - 1}, & \text{if } t \neq 0, \\ 1 - |z|, & \text{if } t = 0, \end{cases} \quad (10)$$

where t is a constant ($-\infty < t < \infty$), called the exponential constant, and z is a standardized parameter representing the distance of the estimated response from its target in units of the maximum allowable deviation. For example, z for a response with a symmetric desirability function is defined as

$$z = \frac{\hat{y}_j(\mathbf{x}) - T_j}{y_j^{\max} - T_j} = \frac{\hat{y}_j(\mathbf{x}) - T_j}{T_j - y_j^{\min}}, \quad \text{for } y_j^{\min} \leq \hat{y}_j(\mathbf{x}) \leq y_j^{\max}. \quad (11)$$

Equation (11) can be easily modified for an asymmetric case. Similarly, z for an STB- or an LTB-type response is defined respectively as follows:

$$z = \frac{\hat{y}_j(\mathbf{x}) - y_j^{\min}}{y_j^{\max} - y_j^{\min}}, \quad \text{for } y_j^{\min} \leq \hat{y}_j(\mathbf{x}) \leq y_j^{\max}, \quad (12)$$

$$z = \frac{y_j^{\max} - \hat{y}_j(\mathbf{x})}{y_j^{\max} - y_j^{\min}}, \quad \text{for } y_j^{\min} \leq \hat{y}_j(\mathbf{x}) \leq y_j^{\max}. \quad (13)$$

z ranges between -1 and 1 for an NTB-type response and between 0 and 1 otherwise. In both cases the desirability function value $d(z)$ achieves its maximum value of 1 when $z = 0$, i.e. $\hat{y}_j(\mathbf{x}) = T_j$, $\hat{y}_j(\mathbf{x}) = y_j^{\min}$ or $\hat{y}_j(\mathbf{x}) = y_j^{\max}$ in equations (11), (12) and (13) respectively. The function $d(z)$ given in equations (10) has been proven to provide a reasonable and flexible representation of human perception (Kirkwood and Sarin, 1980; Moskowitz and Kim, 1993) and is convenient to handle analytically.

The function $d(z)$ can represent many different shapes depending on the exponential constant t ; it is convex, linear and concave when $t < 0$, $t = 0$ and $t > 0$ respectively. As t increases (from $-\infty$ to ∞), $d(z)$ becomes decreasingly convex and increasingly concave. If a convex-shaped desirability function is used, the desirability value changes more rapidly when z is close to 0 (and more slowly when z becomes close to 1) than when using a linear or concave-shaped desirability function. Therefore, using a convex desirability function implies that the deviation of the estimated response from its target value is more critical and hence should be smaller (in units of z) than when using a linear or concave desirability function, to maintain the same degree of satisfaction. (See the points **a**, **b** and **c** at $d(z) = d_0$ in Fig. 2.) Examples of the exponential desirability function with several different t -values are shown in Fig. 2.

A desirability function reflects the DM's belief and is considered by some to be analogous to a utility function in decision analysis (Zimmermann, 1987). A desirability function can be

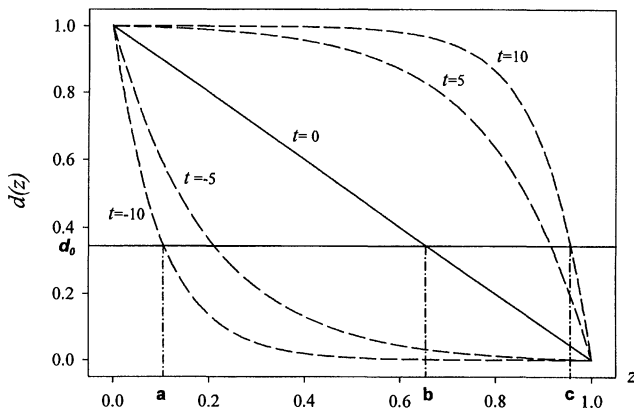


Fig. 2. Exponential desirability functions: $d(z)$ is defined for $-1 \leq z < 1$ for an NTB-type response and for $0 \leq z \leq 1$ otherwise; the graph shows only $0 \leq z \leq 1$; $d(z)$ may have a symmetric or an asymmetric shape for $-1 \leq z \leq 0$

measured by using procedures that are similar to those used for assessing a utility function. For the exponential desirability function case, $d(z)$ can be assessed by identifying just one point on the curve because it has only one unknown parameter t . At an arbitrary point z_0 ($0 < z_0 < 1$), the DM assesses how much the degree of satisfaction (denoted s) would be and then solves the equation $d(z_0) = s$ for t :

$$\frac{\exp(t) - \exp(tz_0)}{\exp(t) - 1} = s, \quad 0 < z_0 < 1, \quad 0 < s < 1. \tag{14}$$

There is no closed form solution to equation (14), and it must be solved numerically.

A related technical issue is the sensitivity of the optimization result to the choice of t —if two DMs produce two different t -values, how will this affect the conclusion? This is a difficult question in general. Some analysis has been done via simulation to address this issue. The findings can be briefly summarized as follows.

- (a) When all $t_j s$ are equal, the choice of t has no effect on the optimal setting \mathbf{x}^* , i.e. the shape of the desirability function does not affect the optimal setting if a common shape is used for all the responses. In fact, this can be proved analytically.
- (b) When the $t_j s$ are not all equal, the optimization result will depend on the $t_j s$, i.e. the optimal setting is determined on the basis of the trade-offs between the responses prescribed by unequal t_j -values. In general, the lower the t_j -value is (less concave or more convex), the higher the influence $\hat{y}_j(\mathbf{x})$ has on the optimal setting determination.

6. Example 2: mechanical properties of JS-SS400 steel

Now, we return to the JS-SS400 steel case introduced in Section 1. An observational study was performed in a major steel company in Korea. 74 data points were collected from the manufacturing process during January–March 1997. A second-order polynomial model was fitted to each of the three responses and then reduced to the best subset model. Note that the approach proposed can use different sets of input variables in the response models, which is not allowed in the KC approach. The best subset models and their R^2 -values are

$$\hat{y}_1(\mathbf{x}) = -101.01 + 1.86x_2 + 2.40x_6 - 0.01x_2^2 - 0.20x_4^2 - 0.01x_5^2 + 0.21x_1x_4 + 0.08x_1x_5 - 0.14x_1x_6 \quad (R^2 = 0.98), \tag{15}$$

$$\hat{y}_2(\mathbf{x}) = 22.59 + 2.58x_3 + 0.43x_5 - 0.004x_2^2 - 0.02x_4^2 - 0.03x_2x_3 + 0.02x_2x_6 - 0.02x_5x_6 \quad (R^2 = 0.94), \tag{16}$$

$$\hat{y}_3(\mathbf{x}) = -1160.11 + 18.71x_1 + 10.83x_2 + 13.53x_5 - 0.52x_1^2 + 0.02x_2^2 - 0.03x_3^2 + 0.01x_5^2 + 0.05x_2x_3 - 0.03x_3x_5 - 0.17x_2x_5 \quad (R^2 = 0.80). \tag{17}$$

The minimum, maximum and target values of each individual fitted response were provided by the production management team of the company. These values are given in Table 2 and were used as the bounds on each response.

Among the three responses, y_1 is considered the most important, followed by y_2 . The production management team agreed on employing a convex, linear and concave desirability function for y_1 , y_2 and y_3 with $t = -3.0, 0.0, 3.0$ respectively. Table 2 also shows the current operating condition and the optimization results. The ‘without R^2 consideration’ portion of Table 2 is discussed next. The ‘with R^2 consideration’ portion will be discussed in Section 7.

Table 2. Best subset models and optimization results of the JS-SS400 steel case

Parameter	Responses		
	y_1	y_2	y_3
<i>Bounds and target</i>			
y_j^{\min}	43.10	26.30	20.00
y_j^{\max}	52.00	48.08	43.67
T_j	47.55	48.08	43.67
<i>Current operating condition $\mathbf{x}^0 = (17.74, 78.08, 15.42, 9.55, 86.75, 63.24)$†</i>			
$y(\mathbf{x}^0)$	48.88	33.79	24.04
<i>Optimization results</i>			
Without R^2 consideration: $(t_1, t_2, t_3) = (-3.0, 0.0, 3.0)$; $\mathbf{x}^* = (18.02, 109.67, 9.57, 12.01, 85.00, 64.00)$			
$\hat{y}_j(\mathbf{x}^*)$	47.72	45.85	34.42
$d_j\{\hat{y}_j(\mathbf{x}^*)\}$	0.88	0.90	0.88
With R^2 consideration: $(t'_1, t'_2, t'_3)‡ = (-2.7, 0.6, 4.4)$; $\mathbf{x}^* = (18.00, 110.00, 9.23, 11.97, 85.00, 64.00)$			
$\hat{y}_j(\mathbf{x}^*)$	47.65	46.28	34.06
$d_j\{\hat{y}_j(\mathbf{x}^*)\}$	0.94	0.94	0.94

† Allowable ranges of x_1-x_6 (x_i^{\min}, x_i^{\max}) are as follows: $x_1 = (0.16, 0.20)$ if $7.00 \leq x_4 \leq 10.00$ and $x_1 = (0.18, 0.22)$ if $10.00 < x_4 \leq 12.70$; $x_2 = (0.70, 0.90)$ if $7.00 \leq x_4 \leq 10.00$ and $x_2 = (0.18, 0.22)$ if $10.00 < x_4 \leq 12.70$; $x_3 = (0.00, 0.03)$; $x_4 = (7.00, 12.70)$; $x_5 = (850, 890)$; $x_6 = (600, 640)$.
 ‡ $t' = t + (1 - R^2)(t^{\max} - t)$ with $t^{\max} = 10$.

6.1. Comparison of current operating condition and optimization results

It is notable that $\hat{y}(\mathbf{x}^*)$ dominates $y(\mathbf{x}^0)$ in all three responses, where $y(\mathbf{x}^0)$ denotes the response values at the current operating condition. The current operating condition was determined on the basis of the engineers' experience, without the aid of formal experimental methodologies. It is clear from the comparison that the current operating condition is far from being optimal. $y_1(\mathbf{x}^0)$ is quite comparable with $\hat{y}_1(\mathbf{x}^*)$, whereas $y_2(\mathbf{x}^0)$ and $y_3(\mathbf{x}^0)$ are significantly worse than their counterparts in $y(\mathbf{x}^*)$. This may be attributed to the fact that y_1 (tensile strength) was of primary concern in setting up the current operating condition because it was impossible in practice to consider all three responses in determining the parameter values.

7. Modified modelling approach: consideration of predictive ability

Neither the KC approach nor the approach presented in Section 3 takes into consideration the predictive ability of the estimated response models. Both approaches implicitly assume that all $\hat{y}_j(\mathbf{x})$ s have the same level of predictive ability. Consequently, the results can be misleading if in fact there is a significant difference in the levels of predictive ability (goodness of fit). The modelling approach proposed can be modified to incorporate the level of predictive ability when this is a concern, by adjusting the shape of the desirability function.

In principle, an estimated response $\hat{y}_j(\mathbf{x})$ with a lower predictive ability should have a smaller effect in the optimization. The discussion in Section 5 indicates that $\hat{y}_j(\mathbf{x})$ with a more concave (or less convex) desirability function has a smaller effect in determining the optimal solution. Conceptually, a lower predictive ability can be translated into a more concave (or less convex) shape of the desirability function. To implement the translation, we need to determine how much adjustment in the shape of the desirability function should be made for a given magnitude of difference in the predictive ability. The predictive ability can be

measured by many different criteria such as R^2 , adjusted R^2 , Akaike's information criterion and the mean-squared error. For simplicity of presentation, we use the well-known R^2 . Other criteria can be used in a similar manner.

To incorporate the predictive ability of a response, we propose to use

$$d'(z) = \begin{cases} \frac{\exp(t') - \exp(t'|z|)}{\exp(t') - 1}, & \text{if } t' \neq 0, \\ 1 - |z|, & \text{if } t' = 0, \end{cases} \tag{18}$$

where $t' = t + (1 - R^2)(t^{\max} - t)$, t is the exponential constant used in equations (10) without considering the predictive ability and t^{\max} is a sufficiently large value of t such that $d(z)$ with t^{\max} is extremely concave and thus has virtually no effect in the optimization. When $R^2 = 1$, $t' = t$ and $d'(z)$ equals $d(z)$ defined in equations (10). However, when $R^2 = 0$, $t' = t^{\max}$ and the corresponding response model would have virtually no effect. In general, when $0 < R^2 < 1$, $t < t' < t^{\max}$ and $d'(z)$ is more concave or less convex than $d(z)$. As mentioned in Kirkwood (1996), realistic values of t will generally have a magnitude between -10 and 10 . We suggest $t^{\max} = 10$ for practical use.

In summary, the desirability function is assessed in a two-step procedure, namely the basic desirability function $d(z)$ in the first step and the modified desirability function $d'(z)$ in the second step. $d(z)$ is determined solely on the basis of the generic importance of the response. Then, the predictive ability is taken into account to transform $d(z)$ into $d'(z)$.

Fig. 3 illustrates the shape of $d'(z)$ when $R^2 = 0.5$ for three different $d(z)$ s, namely $t = -3.0$, 0.0 and 3.0 in Fig. 3(a), Fig. 3(b) and Fig. 3(c) respectively. In all three cases, the $d'(z)$ s are more concave than the corresponding $d(z)$ s, but with different degrees. As the t -value of $d(z)$ becomes lower, the change in t due to an imperfect R^2 -value becomes bigger (i.e. $\Delta t = t' - t = 6.5, 5.0$ and 3.5 in Fig. 3(a), Fig. 3(b) and Fig. 3(c) respectively). This implies that, as the desirability function of a response becomes less concave (or more convex), its use should be justified by a higher R^2 -value of the corresponding estimated response. This is to avoid the optimization algorithm's placing unduly high priority on an estimated response model which is not reliable. Hence, in the adjustment scheme proposed, the t' -value becomes more rapidly 'inflated' by a unit decrease in R^2 as the basic t -value becomes lower.

7.1. Mechanical properties of JS-SS400 steel

We illustrate the modified modelling approach by using the case discussed in Section 6. In this case, $\hat{y}_3(\mathbf{x})$ has a notably lower R^2 -value than do $\hat{y}_1(\mathbf{x})$ and $\hat{y}_2(\mathbf{x})$. (The R^2 -values for $\hat{y}_1(\mathbf{x})$, $\hat{y}_2(\mathbf{x})$ and $\hat{y}_3(\mathbf{x})$ are 0.98, 0.94 and 0.80 respectively.) On the basis of the R^2 -values, modified desirability functions $d'(z)$ are constructed. As shown in Table 2, the modified exponential coefficients t' are $-2.7, 0.6$ and 4.4 for y_1, y_2 and y_3 respectively. $d(z)$ s and the corresponding $d'(z)$ s are depicted in Fig. 4.

When the R^2 -difference is taken into account, $\hat{y}_1(\mathbf{x}^*)$ has improved from 47.72 to 47.65 (i.e. has moved closer to the target value by 0.07). This is because $d'(z)$ for y_1 is now even more convex, in a relative sense, than other $d'(z)$ s, indicating that a higher priority has been placed on y_1 in the optimization process compared with the 'without R^2 consideration' case. In contrast, $\hat{y}_3(\mathbf{x}^*)$ has been lowered because of its low R^2 . The difference between the optimization results without and with R^2 consideration increases as the difference in the R^2 -values among the responses increases.

It is certainly possible to envision situations where the desirability value never fell to 0, because it was not absolutely essential to the overall satisfaction. Even in such a case, the

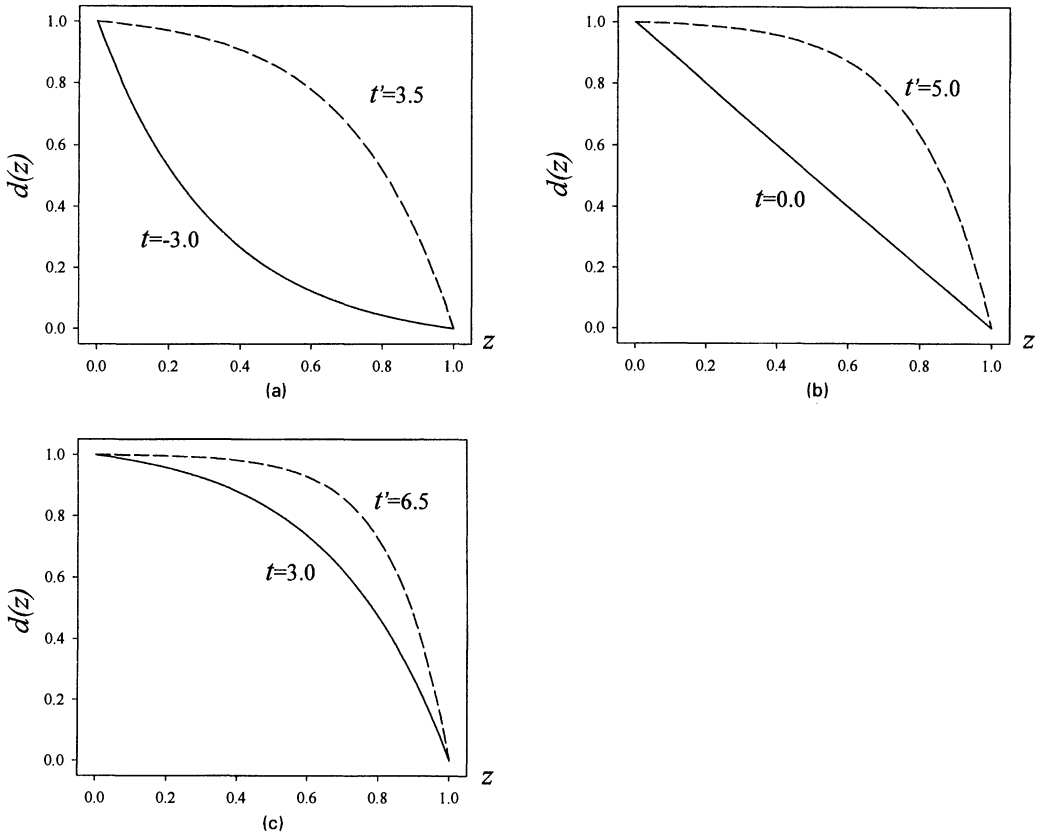


Fig. 3. Basic desirability functions $d(z)$ (—) versus modified desirability functions $d'(z)$ (---) when $R^2 = 0.5$: (a) $t = -3.0$; (b) $t = 0.0$; (c) $t = 3.0$

modification idea discussed above can be equally applied, namely, regardless of the shape of $d(z)$, $d'(z)$ would be more concave than the original $d(z)$ (assuming that $R^2 < 1$) and thus positioned between $d(z)$ and the extremely concave desirability function (i.e. $d(z)$ with t^{\max}), with the starting-point ($d(z)$ at $z = 0$) and the ending point ($d(z)$ at $z = 1$) remaining fixed.

Table 3 compares the KC approach and the modified modelling approach discussed in this section in terms of the optimization criterion, assumptions and model characteristics. In contrast with the KC approach, the approach proposed does not require any assumptions regarding the form or degree of the estimated response models and the existence of linear dependences between the responses. Moreover, it takes into consideration the difference in the predictive ability and the relative priority among the estimated models through an adjustment of the shape of the desirability function.

8. Conclusions

An alternative modelling approach to optimize the multiresponse system, based on maximizing exponential desirability functions, has been presented. The approach proposed aims to identify the setting of input variables to maximize the overall minimal level of satisfaction with respect to all the responses.

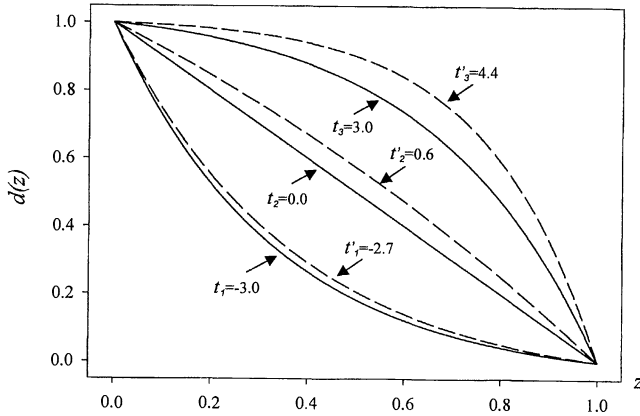


Fig. 4. Basic desirability functions $d(z)$ (—) versus modified desirability functions $d'(z)$ (---) for the JS-SS400 steel case (for y_1 (NTB type), only the right-hand half of the desirability function is shown)

Table 3. Comparison of the KC approach and the approach proposed

	KC approach	Approach proposed
Optimization criterion	Minimize the distance of $\hat{y}_j(\mathbf{x})$ from ϕ (being closest to the ideal point)	Maximize the overall degree of satisfaction of all responses (achieving an optimal balance)
Model assumptions		
Response models	Each response should be of the same functional form and use the same design	Each response may have different functional form and different set of input variables
Dependence between responses	Dependence should be removed in advance (dependence is unidentifiable in general)	No assumption needed (dependence does not matter)
Prediction ability of responses	Assume equal prediction ability for all individual response modelling	Different prediction ability can be incorporated into the shape of desirability function
Relative weights among responses	Relative weights are assumed to be equal	Relative weights can be incorporated into the shape of desirability function

The approach proposed does not require any assumptions regarding the form or degree of the estimated response models and the existence of linear or non-linear dependences between the responses (although the usual assumptions on the random-error terms and the exponential shape of the desirability function are still needed). Moreover, it takes into consideration the difference in the predictive ability and the relative priority among the estimated models through an adjustment of the shape of the desirability function. Therefore, the approach proposed enables practitioners to overcome some limitations of the existing approaches, e.g. requiring all response models to be of the same functional form, use of the same design, being dependent on knowing the variance-covariance matrix and being unable to take into account the size of the prediction variance (Khuri, 1996).

The model proposed can certainly be modified by users for their specific needs. In particular, the R^2 -value was used as a measure of the predictive ability of a response model.

However, any performance measure other than R^2 can be employed as appropriate. In Section 7, our model proposed that the modified exponential constant t' be determined by $t + (1 - R^2)(t^{\max} - t)$, which is essentially a linear function of R^2 (or whatever performance measure the users choose to employ). Different functional forms of R^2 can be devised to accelerate or decelerate the adjustment of the t' -value with the change in R^2 -value. All computations associated with the optimization approach proposed can be done using any general algorithm for a non-linear problem.

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References

- Bellman, R. and Zadeh, L. (1970) Decision-making in a fuzzy environment. *Management Sci.*, **17**, B141–B164.
- Box, G. E. P. and Draper, N. R. (1987) *Empirical Model Building and Response Surfaces*. New York: Wiley.
- Chameau, J. and Santamarina, J. (1987) Membership functions I: Comparing methods of measurements. *Int. J. Approx. Reasoning*, **1**, no. 3, 1–15.
- Church, A. (1978) Optimizing properties of formulations. *Technical Report 1*. Research Division, General Tire & Rubber Company.
- Derringer, G. (1994) A balancing act: optimizing a product's properties. *Qual. Prog.*, 51–58.
- Derringer, G. and Suich, R. (1980) Simultaneous optimization of several response variables. *J. Qual. Technol.*, **12**, 214–219.
- Harrington, E. (1965) The desirability function. *Industrial Qual. Control*, 494–498.
- Hillier, F. and Lieberman, G. (1995) *Introduction to Mathematical Programming*, 2nd edn. New York: McGraw Hill.
- Inglis, I., Forkman, B. and Lazarus, J. (1997) Free food or earned food?: a review and fuzzy model of contra-freeloading. *Anim. Behav.*, **53**, 1171–1191.
- Khuri, A. (1996) Multiresponse surface methodology. In *Handbook of Statistics: Design and Analysis of Experiments* (eds A. Ghosh and C. R. Rao), vol. 13, pp. 377–406. Amsterdam: North-Holland.
- Khuri, A. and Conlon, M. (1981) Simultaneous optimization of multiple responses represented by polynomial regression functions. *Technometrics*, **23**, 363–375.
- Khuri, A. and Cornell, J. (1996) *Response Surfaces: Designs and Analyses*. New York: Dekker.
- Kirkwood, C. W. (1996) *Strategic Decision Making*. Belmont: Duxbury.
- Kirkwood, C. W. and Sarin, R. K. (1980) Preference conditions for multiattribute value functions. *Ops Res.*, **28**, 225–232.
- Kwon, O. and Baik, D. (1989) A technology for the prediction and control of microstructural changes and mechanical properties in steel. *Technical Paper*. Research Institute of Industrial Science and Technology, Pohang.
- Lavolette, M., Seaman, J., Barrett, J. and Woodall, W. (1995) A probabilistic and statistical view of fuzzy methods. *Technometrics*, **37**, 249–261.
- Lind, E., Goldin, J. and Hickman, J. (1960) Fitting yield and cost response surfaces. *Chem. Engng Prog.*, **56**, 62–68.
- Moskowitz, H. and Kim, K. (1993) On assessing the H value in fuzzy linear regression. *Fuzzy Sets Syst.*, **58**, 303–327.
- Murty, K. (1976) *Linear and Combinatorial Programming*. New York: Wiley.
- Zimmermann, H. J. (1987) *Fuzzy Sets, Decision Making, and Expert Systems*. Boston: Kluwer.